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FINAL AFOSR REPORT (Dec. 1, 2008-Nov. 30, 2011)

I. Grant Title:

Vacuum Ultraviolet Laser Probe of Chemical Dynamics of Aerospace Relevance

II. Principal Investigator and Address

Cheuk-Yiu Ng

Address: Department of Chemistry
University of California at Davis
Davis, California 95616

III. Contract Number: FA9550-09-1-0054

IV. Objective:

A primary goal of this research program is to provide pertinent information about the energetics, photochemistry, and chemical dynamics of spacecraft effluents, including H_2O , NH_3 , hydrazine (N_2H_4), monomethylhydrazine, and unsymmetrical dimethylhydrazine. By using the unique VUV laser facilities developed in our laboratory, we plan to perform high-resolution photodissociation, photoionization, and photoelectron studies of these molecules, and to examine their chemical interactions with major atmospheric ions, aiming to identify possible sources of optical emission signatures that can be used for reliable tracking and detection of spacecraft maneuvers and rocket launches. Rovibrationally excited $\text{O}_2^+(\text{X}^2\Pi_{3/2,1/2}; v^+)$, $\text{O}_2^+(\text{a}^4\Pi_u; v^+)$ and $\text{N}_2^+(\text{X}^2\Sigma_g^+; v^+)$ ions are known to be among the major ionic species produced by solar VUV photoionization and electron impact ionization. These excited O_2^+ and N_2^+ species are long-lived and expected to play a significant role in atmospheric reactions. Nevertheless, reaction cross sections involving these rovibrational excited ions with atmospheric neutrals remain mostly unknown. We have successfully developed a novel, high-resolution VUV laser pulsed field ionization-photoion (PFI-PI) scheme for the preparation of rovibrationally selected $\text{O}_2^+(\text{X}^2\Pi_{3/2,1/2}; v^+=0-38, N^+)$, $\text{O}_2^+(\text{a}^4\Pi_u; v^+=18, N^+)$, and $\text{N}_2^+(\text{X}^2\Sigma_g^+; v^+=9, N^+)$ ions with high intensities and high laboratory kinetic energy resolutions ($\Delta E_{\text{lab}} = 50 \text{ meV}$), allowing the measurement of reactions cross sections down to thermal energies. We proposed to conduct detailed absolute total cross section measurements for reactions between these state-selected diatomic ions and atmospheric neutrals, including atomic neutrals, Ar, $\text{O}(^3\text{P})$, and $\text{O}(^1\text{D})$, diatomic neutrals, H_2 , O_2 , N_2 , NO, and CO, and polyatomic neutrals, HCN, H_2O , CO_2 , NH_3 , CH_4 , C_2H_2 , N_2H_4 and C_2H_4 . Particular emphasis will be placed on the reaction dynamics involving reactant ions in highly vibrationally excited states. These state-resolved absolute total cross sections obtained as a function of kinetic energy are valuable for modeling aerospace environments using the Direct Simulation Monte Carlo and Particles in Cell methods. Environments of interest to the Air Force include nonequilibrium, hypersonic air plasma, such as those associated with communications blackout of reentry space vehicles and the plasmas of electric propulsion thrusters. They are also important for accurate simulation of density profiles of electron, ions, and neutrals in planetary atmospheres.

V. Technical developments

1. Technique for the preparation of State-selected ions

By employing an electric field pulsing scheme for vacuum ultraviolet (VUV) laser pulsed field ionization-photoion (PFI-PI) measurements, we have been able to prepare a rovibrationally selected PFI-PI beam of $\text{N}_2^+(v^+=1, N^+)$ with not only high intensity and high quantum state purity, but also high kinetic energy resolution. This represents a technical breakthrough for the preparation of state-selected ions for ion-molecule reaction studies. This work has just been published as a *communication* in the *Journal of Chemical Physics* [see Chang et al., “Communication: Rovibrationally selected study of the $\text{N}_2^+(\text{X}; v^+ = 1, N^+ = 0-8) + \text{Ar}$ charge transfer reaction using the vacuum ultraviolet laser pulsed field ionization-photoion method”, *J. Chem. Phys.* **134**, 201105 (2011)].

Using the $\text{N}_2^+(X^2\Sigma_g^+; v^+) + \text{Ar}$ charge transfer process as a demonstration reaction, we show that the low ΔE_{lab} spread for the rovibronically selected N_2^+ beam achieved here allows the cross section measurements to be extended down to thermal energies. We compare in Fig. 4 the charge transfer cross sections for $\text{N}_2^+(v^+=1, N^+=0-8)$ at $E_{\text{cm}}=0.04-10.00$ eV obtained in this study with previous theoretical and experimental results, which include cross sections converted from reported rate coefficients. The previous experimental and theoretical results are scattered and are mostly higher than the present measurements. However, the cross section curve observed here is in excellent agreement with the theoretical predictions based on the Landau-Zener-Stückelberg formulism and the *ab initio* potential energy surface calculated for the $[\text{N}_2+\text{Ar}]^+$ reaction system.

In addition to achieving the high kinetic energy resolution, the internal energy selection by the VUV laser PFI-PI method has made possible the examination of the rotational effect on the charge transfer cross section.

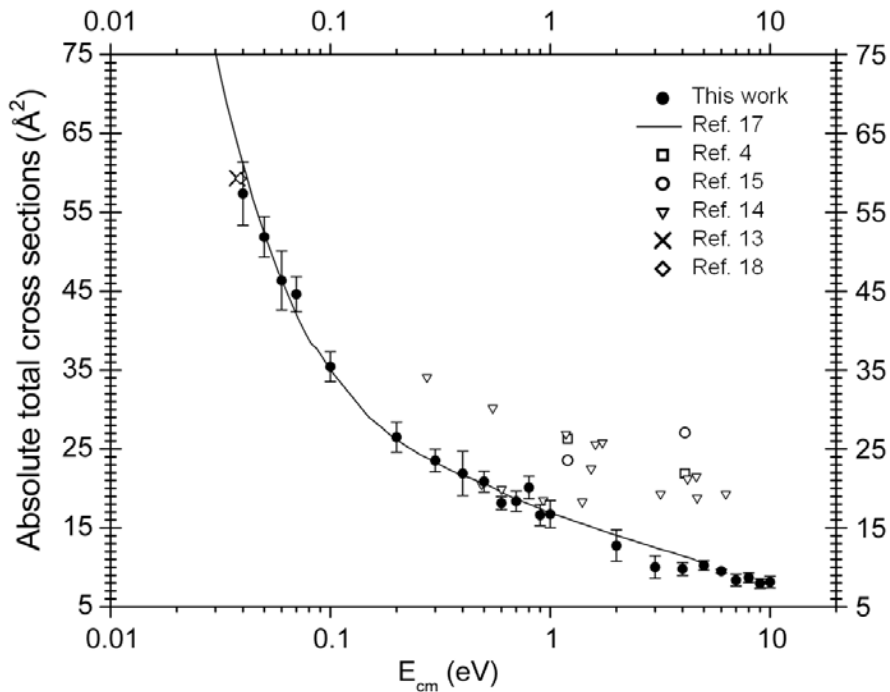


Figure 1. Comparison of $\sigma(v^+=1, N^+=0-8)$ values measured at $E_{\text{cm}}=0.04-10.00$ eV, obtained here with previous theoretical predictions and experimental results, which include cross sections converted from rate constant measurements.

After this successful demonstration experiment, we are currently working on the ion-molecule reactions $\text{N}_2^+(v^+=0-2, N^+=0-8) + \text{CH}_4$ (H_2O , and C_2H_4). Interesting preliminary results on the vibrational effect for the reaction cross sections of these processes have been obtained.

2. VUV photodissociation by VUV photoionization probe

We have demonstrated that the VUV photodissociation dynamics of N_2 and CO_2 can be studied using VUV photoionization with time-sliced velocity-

mapped ion imaging (VUV-PI-VMI) detection. This represents the first experimental study employing two tunable VUV lasers. This work has just published as a *communication* in *Journal of Chemical Physics* [see Pan et al., “Communication: Vacuum ultraviolet laser photodissociation studies of small molecules by the vacuum ultraviolet laser photoionization time-sliced velocity-mapped ion imaging method”, *J. Chem. Phys.* **135**, 071101 (2011)].

In the case of CO_2 , we show for the first time that $\text{O}(^1\text{D})$ atom is produced with $\text{CO}(^1\Sigma^+)$ at 92.21 nm as depicted in Fig. 2.

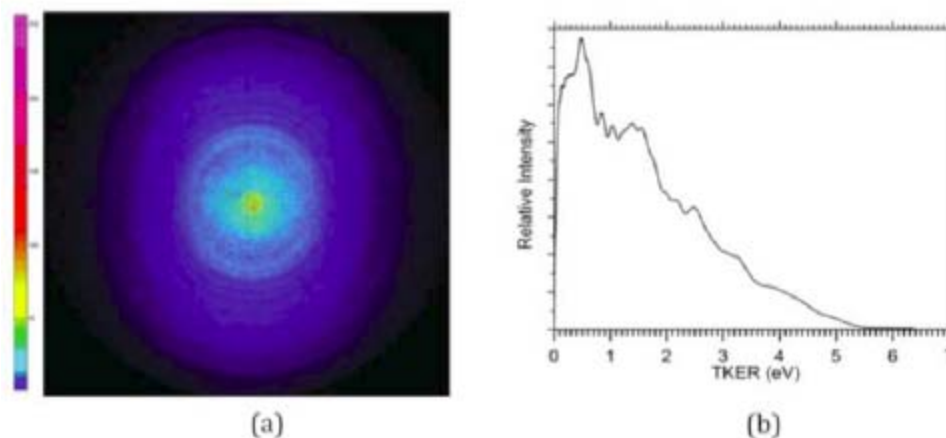


Figure 2. Photodissociation of CO_2 at 108451.5 cm^{-1} . Oxygen atoms in the $\text{O}(^1\text{D}_2)$ state are detected via the autoionization transition $2s^22p^3(^2\text{D}_{3/2}^o)3d\ ^1\text{D}_2 \leftarrow \text{O}(^1\text{D}_2)$, (a) The sliced VUV-PI-VMI-image and (b) the $P(E_T)$ derived from the image.

Currently, the ion-imaging apparatus is used for the VUV-photodissociation and VUV-photoionization studies of H_2O , NH_3 , and N_2H_4 .

3. High-resolution near VMI-TPE detection

We have recently implemented the VUV laser VMI-photoelectron imaging technique with the ion-imaging apparatus by adding appropriate μ -metal shields to the velocity-mapped ion-imaging apparatus. We found that this method can provide an energy resolution close to that achieved in VUV-PFI-PE measurements if the VUV photoionization energy is set near the photoelectron band of interest.

Further to this development, we have successfully established the VUV laser VMI-threshold photoelectron imaging method for high-resolution TPE measurements, achieving an electron energy resolution of 2 cm^{-1} (FWHM). The TPE measurements are made by gating the TPE signal imaged at the center of the imaging detector. Figure 3 compares the VUV-TPE imaging (VUV-VMI-TPE) spectrum (upper curve) thus obtained with the VUV-PFI-PE spectrum (lower curve) of $\text{C}_6\text{H}_5\text{Cl}$ in the energy range of 9.06-9.48 eV. The energy resolution for the VUV-PFI-PE measurement has been measured to be $1.5\text{-}2.0\text{ cm}^{-1}$ (FWHM). Since the FWHMs of all the VUV-VMI-TPE bands are nearly identical to those of the corresponding VUV-PFI-PE bands, we conclude that the energy resolution achieved in this VUV-TPEI measurement is 2 cm^{-1} (FWHM).

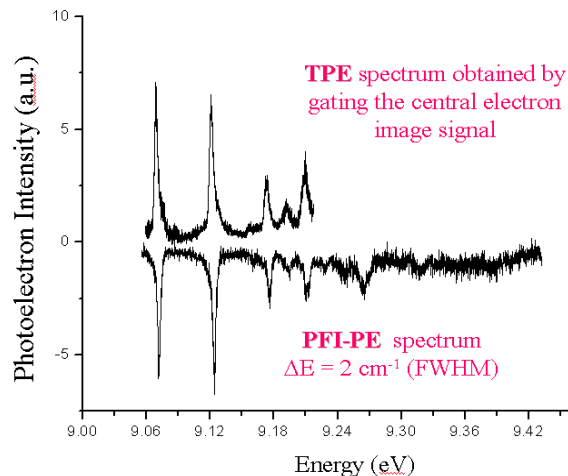


Figure 3. Comparison of the VUV-TPEI spectrum (upper spectrum) with the VUV-PFI-PE spectrum (lower spectrum), showing that the resolution achieved for the VUV-TPE-EI measurement is close to 2 cm^{-1} (FWHM) observed in VUV-PFI-PE measurements.

VI. Selected scientific findings

1. Kai-Chung Lau, Yih-Chung Chang, Xiaoyu Shi, and C. Y. Ng, “High-level *ab initio* predictions of the ionization energy, bond dissociation energies and heats of formations for nickel carbide (NiC) and its cation (NiC^+)”, *J. Chem. Phys.* **133**, 114304 (2010).

The ionization energy (IE) of NiC and the 0 K bond dissociation energies (D_0) and heats of formation at 0 K (ΔH°_{f0}) and 298 K (ΔH°_{f298}) for NiC and NiC^+ are predicted by the wavefunction based CCSDTQ(Full)/CBS approach and the multi-reference configuration interaction (MRCI) method with Davidson correction (MRCI+Q). The CCSDTQ(Full)/CBS calculations presented here

involve the approximation to the complete basis set (CBS) limit at the coupled cluster level up to full quadruple excitations along with the zero-point vibrational energy (ZPVE), high-order correlation (HOC), core-valence electronic (CV), spin-orbit coupling (SO), and scalar relativistic effect (SR) corrections. The present calculations provide the correct symmetry predictions for the ground states of NiC and NiC⁺ to be ¹Σ⁺ and ²Σ⁺, respectively. The CCSDTQ(Full)/CBS IE(NiC) = 8.355 eV is found to compare favorably with the experimental IE value of 8.37209 ± 0.00006 eV. The predicted IE(NiC) value at the MRCI+Q/cc-pwCV5Z level, including the ZPVE, SO, and SR effects is 8.00 eV, which is 0.37 eV lower than the experimental value. This work together with the previous experimental and theoretical investigations supports the conclusion that the CCSDTQ(Full)/CBS method is capable of providing reliable IE predictions for 3d-transition metal carbides, such as FeC and NiC. Furthermore, the CCSDTQ(Full)/CBS calculations give the prediction of D₀(Ni–C) – D₀(Ni⁺–C) = 0.687 eV, which is also consistent with the experimental determination of 0.73221 ± 0.00006 eV, whereas the MRCI+Q calculations predict a significantly lower value of 0.39 eV for D₀(Ni–C) – D₀(Ni⁺–C). The analysis of the correction terms shows that the CV and valence-valence electronic correlations beyond CCSD(T) wavefunction and the relativistic effect make significant contributions to the calculated thermochemical properties of NiC/NiC⁺. For the experimental D₀ and ΔH⁰_{f0} values of NiC/NiC⁺, which are not known experimentally, we recommend the CCSDTQ(Full)/CBS predictions [D₀(Ni–C) = 4.047 eV, D₀(Ni⁺–C) = 3.361 eV, ΔH⁰_{f0}(NiC) = 749.0 kJ/mol and ΔH⁰_{f0}(NiC⁺) = 1555.1 kJ/mol].

2. C.-S. Lam, Hailing Wang, Yubtao Xu, “A Vacuum-Ultraviolet Laser Pulsed Field Ionization-Photoelectron Study of Sulfur Monoxide (SO) and its Cation (SO⁺)”, *J. Chem. Phys.* **134**, 144304 (2011).

Vacuum ultraviolet (VUV) laser pulsed field ionization-photoelectron (PFI-PE) spectroscopy has been applied to the study of the sulfur monoxide radical (SO) prepared by using a supersonically cooled radical beam source based on the 193 nm excimer laser photodissociation of SO₂. The vibronic VUV-PFI-PE bands for the photoionization transitions SO⁺(X²Π_{1/2}; v⁺ = 0) ← SO(X³Σ[−]; v = 0) and SO⁺(²Π_{3/2}; v⁺ = 0) ← SO(X³Σ[−]; v = 0) have been recorded. On the basis of the semi-empirical simulation of rotational branch contours observed in these PFI-PE bands, we have obtained highly precise ionization energies (IEs) of 83 034.2 ± 1.7 cm^{−1} (10.2949 ± 0.0002 eV) and 83 400.4 ± 1.7 cm^{−1} (10.3403 ± 0.0002 eV) for the formation of SO⁺(X²Π_{1/2}; v⁺ = 0) and SO⁺(²Π_{3/2}; v⁺ = 0), respectively. The present VUV-PFI-PE measurement has enabled the direct determination of the spin-orbit coupling constant (A₀) for SO⁺(X²Π_{1/2,3/2}) to be 365.36 ± 0.12 cm^{−1}. We have also performed high-level *ab initio* quantum chemical calculations using the wavefunction based CCSDTQ(Full)/CBS approach, which involves the approximation to the complete basis set (CBS) limit at the coupled cluster level up to full quadruple excitations. The zero-point vibrational energy correction, the core-valence electronic correction, the spin-orbit coupling, and the high-level correction are included in the calculation. The IE[SO⁺(X²Π_{1/2,3/2})] and A₀

predictions thus obtained are found to be in remarkable agreement with the experimental determinations.

VII. Personnel Supported:

- | | | |
|----|-------------------------|---|
| 1. | Professor Cheuk-Yiu Ng: | Principal investigator |
| 2. | Dr. Yih-Chung Ian Chang | Postdoctoral associate |
| 3. | Mr. Yuntao Xu: | Graduate student (4 th year student) |
| 4. | Mr. Zhou Lu | Graduate student (2 nd year student) |

VIII. Publications (2009-present):

1. C. Y. Ng, "Spectroscopy and Dynamics of Neutrals and Ions by high-resolution infrared-vacuum ultraviolet photoionization and photoelectron methods", in *"Frontiers of Molecular Spectroscopy"*, edited by Jaan Laane (Elsevier Science and Technology, 2009) Chap. 19, page 659-691.
3. B. Reed, C.-S. Lam, Y.-C. Chang, X. Xing, and C. Y. Ng, "A high-resolution photoionization study of ⁵⁶Fe using vacuum ultraviolet laser", *Astrophys. J.*, **693**, 940 (2009).
4. Y.-C. Chang, C.-S. Lam, B. Reed, K.-C. Lau, H. T. Liou, and C. Y. Ng, "Rovibronically selected and resolved two-color laser photoionization and photoelectron study of the iron carbide cation", *J. Phys. Chem. A* (invited), **113**, 4242 (2009).
5. Kai-Chung Lau, Yih-Chung Chang, Chow-Sheng Lam, and C. Y. Ng, "High-level *ab initio* predictions of the ionization energy, bond dissociation energies and heats of formations for Iron carbide (FeC) and its cation (FeC⁺)", *J. Phys. Chem. A* (invited), **113**, 14321 (2009).
6. Kai-Chung Lau, Yih-Chung Chang, Chow-Sheng Lam, and C. Y. Ng, "High-level *ab initio* predictions of the ionization energy, bond dissociation energies and heats of formations for Iron carbide (FeC) and its cation (FeC⁺)", *J. Phys. Chem. A* (invited), **113**, 14321 (2009).
7. Yih-Chung Chang, Xiaoyu Shi, Kai-Chung Lau, Qingzhu Yin, and C. Y. Ng, "Rovibronically selected and resolved two-color laser photoionization and photoelectron study of the nickel carbide cation", *J. Chem. Phys.* **133**, 054310 (2010).
8. Kai-Chung Lau, Yih-Chung Chang, Xiaoyu Shi, and C. Y. Ng, "High-level *ab initio* predictions of the ionization energy, bond dissociation energies and heats of formations for nickel carbide (NiC) and its cation (NiC⁺)", *J. Chem. Phys.* **133**, 114304 (2010).
9. C.-S. Lam, Hailing Wang, Yubtao Xu, "A Vacuum-Ultraviolet Laser Pulsed Field Ionization-Photoelectron Study of Sulfur Monoxide (SO) and its Cation (SO⁺)", *J. Chem. Phys.* **134**, 144304 (2011).
10. Yih Chung Chang, Hong Xu, Yuntao Xu, Zhou Lu, Yu-Hui Chiu, Dale J. Levandier and C. Y. Ng. "Communication: Rovibrationally selected study of the

- $\text{N}_2^+(X; v^+ = 1, N^+ = 0-8) + \text{Ar}$ charge transfer reaction using the vacuum ultraviolet laser pulsed field ionization-photoion method”, *J. Chem. Phys.* **134**, 201105 (2011).
11. Yan Pan, Hong Gao, Lei Yang, Jingang Zhou, C. Y. Ng, and W. M. Jackson, “*Communication*: VUV laser photodissociation studies of small molecules by the VUV laser photoionization time-sliced velocity-mapped ion imaging method”, *J. Chem. Phys.* **135**, 071101 (2011). Among the top 20 most download JCP articles in Aug., 2011.
 12. Hong Gao, Lei Yang, Yan Pan, Jingang Zhou, C. Y. Ng, and W. M. Jackson, “Time-sliced velocity-mapped imaging studies of the predissociation of single ro-vibronic energy levels of N_2 in the extreme ultraviolet region using VUV photoionization”, *J. Chem. Phys.* **135**, 134319 (2011).
 13. Hong Gao, Yuntao Xu, Lei Yang, Chow-Shing Lam, Hailing Wang, Jingang Zhou, and C. Y. Ng, “High-resolution threshold photoelectron study of the propargyl radical by the vacuum ultraviolet laser velocity-map imaging method”, *J. Chem. Phys.* **135**, 224304 (2011).
 14. Hong Gao, Yu Song, Lei Yang, Xiaoyu Shi, Qingzhu Yin, C. Y. Ng, and W. M. Jackson, “*Communication*: Branching ratio measurement in the predissociation of $^{12}\text{C}^{16}\text{O}$ by time-slice velocity-map ion imaging in the vacuum ultraviolet region”, *J. Chem. Phys.* **135**, 221101 (2011).
 15. Kai-Chung Lau and C. Y. Ng, “Accurate *ab initio* predictions of ionization energies of propargyl radical: revisited”, *J. Chem. Phys.* **135**, 246101 (2011).
 16. Hong Gao, Yang Pan, Lei Yang, Jingang Zhou, C. Y. Ng, and W. M. Jackson, “Time-sliced velocity-map ion imaging studies of the photodissociation of NO in the extreme vacuum ultraviolet (EUV) region”, *J. Chem. Phys.* **136**, 134302 (2012).
 17. Xiaoyu Shi, Huang Huang, Brian Jacobson, Yih-Chung Chang, Qing-Zhu Yin, and C. Y. Ng, “A high-resolution photoionization and photoelectron study of ^{58}Ni using a vacuum ultraviolet laser”, *Astrophys. J.* **747**, 20 (2012).

IX. Interactions/Transitions:

A. Invited talks at workshops, conferences, and seminars (2009-present)

1. C. Y. Ng, “Why Modern Universities Should Emphasize Basic Science Research”, *Public Lecture* sponsored by the 2008/2009 Siu Lien Wong Visiting Fellow Program, Annual Education Conference: Basic Science Research – Role in Contemporary Society,” Chung Chi College, The Chinese University of Hong Kong, Feb. 28, 2009.
2. C. Y. Ng, “Undergraduate Experience: its insights for future career development”, *Public Lecture* (Assembly Talk) sponsored by the 2008/2009 Siu Lien Wong Visiting Fellow Program, Chapel, Chung Chi College, The Chinese University of Hong Kong, Feb. 27, 2009.
3. C. Y. Ng, “Role of Chinese Scientists in Advocating Science Research in China”, *Public Lecture* sponsored by the 2008/2009 Siu Lien Wong Visiting Fellow

- Program, Chung Chi College, The Chinese University of Hong Kong, Feb. 25, 2009.
4. C. Y. Ng, "Science and Religion: Their Role in the Promotion of Democracy", *Public Lecture* sponsored by the 2008/2009 Siu Lien Wong Visiting Fellow Program, Theology Building, Chung Chi College, The Chinese University of Hong Kong, March 5, 2009.
 5. C. Y. Ng, "Spectroscopy and Dynamics of Neutrals and Ions by High-Resolution IR-VUV Laser Photoion-Photoelectron Methods", JILA and Department of Chemistry, University of Colorado, Boulder, CO., April 10, 2009.
 6. C. Y. Ng, "Rovibronically Selected and Resolved Photoionization and Photoelectron Studies Using Two-Color Infrared-Vacuum Ultraviolet Laser Pulsed Field Ionization Methods", Plenary Lecture, "25th Symposium on Chemical Kinetics and Dynamics", Omiya, Japan, June 1-3, 2009.
 7. C. Y. Ng, "Spectroscopy, energetics, and reaction dynamics of ions and neutrals by high-resolution VUV photoion-photoionization methods", Tokyo University of Science, Tokyo, Japan, June 4, 2009.
 8. C. Y. Ng, "Spectroscopy, energetics, and reaction dynamics of ions and neutrals by high-resolution VUV photoion-photoionization methods", Cluster Research Laboratory, Toyota Technological Institute in East Tokyo Laboratory, Japan, June 5, 2009.
 9. C. Y. Ng, "Spectroscopy, energetics, and reaction dynamics of ions and neutrals by high-resolution VUV photoion-photoionization methods", Kyoto University, June 8, 2009.
 10. C. Y. Ng, "Spectroscopy, energetics, and reaction dynamics of ions and neutrals by high-resolution VUV photoion-photoionization methods", Institute for Molecular Sciences, Okazaki, Japan, June 11, 2009.
 11. C. Y. Ng, "Spectroscopy and Dynamics of Neutrals and Ions by High-Resolution IR-VUV Laser Photoion-Photoelectron Methods", Institute for Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan, June 15, 2009.
 12. C. Y. Ng, "Spectroscopy, energetics, and reaction dynamics of ions and neutrals by high-resolution VUV photoion-photoionization methods", Genome Research Center, Academia Sinica, Taipei, Taiwan, June 16, 2009.
 13. C. Y. Ng, "Spectroscopy and Dynamics of Neutrals and Ions by High-Resolution IR-VUV Laser Photoion-Photoelectron Methods", Workshop on "Vibrational Dynamics", Telluride Summer Research Center, Colorado, July 20-24, 2009.
 14. C. Y. Ng, "Photoionization and photoelectron studies of transition-metal-containing molecules using single-photon and two-color laser excitation schemes", The 6th Joint Meeting of Overseas Physics Association: International Conference on Physics Education and Frontier Physics", Lanzhou, China, August 3-7, 2009.
 15. C. Y. Ng, "Spectroscopy and Dynamics of Neutrals and Ions by High Resolution VUV and IR-VUV Laser Photoionization and Photoelectron Methods", 11th National Meeting in Chemical Kinetics and Dynamics, Yangtze River Cruises, August 13-17, 2009.
 16. "Spectroscopy and Dynamics of Neutrals and Ions by High-Resolution IR-VUV Laser Photoion-Photoelectron Methods", Symposium on 25 years of ZEKE

- Spectroscopy, ACS Meeting, Washington D. C., Aug. 16-20, 2009. Presented by Xi Xing.
17. C. Y. Ng, "Spectroscopy and Dynamics of Neutrals and Ions by High-Resolution IR-VUV Laser Photoion-Photoelectron Methods", Asiloma Spectroscopy Conference, American Society for Mass Spectrometry, Asilomar Conference Center, Oct. 16-19, 2009.
 18. C. Y. Ng, "Spectroscopy, Energetics, and Reaction Dynamics of Neutrals and Ions by High-Resolution VUV Photoionization and Photoelectron Methods", Shanghai Light Source, Shanghai, China, Dec. 1, 2009.
 19. C. Y. Ng, "Spectroscopy, Energetics, and Reaction Dynamics of Neutrals and Ions by High-Resolution VUV Photoionization and Photoelectron Methods" FUNSOM Lab., Soochow University, China, Dec. 2, 2009.
 20. C. Y. Ng, "Vacuum ultraviolet Probes of Spectroscopy and Dynamics", 57th Western Spectroscopy Association, Asiloma Conference, Feb. 3-5, 2010.
 21. C. Y. Ng, "Spectroscopy, Energetics, and Reaction Dynamics of Neutrals and Ions by High-Resolution VUV Photoionization and Photoelectron Methods", Department of Chemistry, Xiamen University, March 24, 2010.
 22. C. Y. Ng, "Two-Color Laser Photoion-Photoelectron Studies of Transition Metal-Containing Species", Department of Chemistry, Peking University, May 14, 2010.
 23. C. Y. Ng, "Workshop on Ion traps and Ion Guides", Telluride Summer Research Center, Colorado, July 19-23, 2010.
 24. C. Y. Ng, "Spectroscopy, Energetics, and Dynamics of Neutrals and Ions by High-Resolution VUV Photoionization and Photoelectron Methods", East China Normal University, Aug. 2010.
 25. C. Y. Ng, "Commencement Speech", 85th Anniversary Graduation Commencement, Clementi Secondary School, Hong Kong, Nov. 5, 2010.
 26. C. Y. Ng, "Spectroscopy, Energetics, and Dynamics of Neutrals and Ions by High-Resolution VUV Photoionization and Photoelectron Methods", Modern Optics and Spectroscopy Seminar Series, Harrison Spectroscopy Lab., MIT, Nov. 16, 2010.
 27. C. Y. Ng, "Spectroscopy, Energetics, and Dynamics of Neutrals and Ions by High-Resolution VUV Photoionization and Photoelectron Methods", Department of Chemistry, Brown University, Nov. 18, 2010.
 28. C. Y. Ng, "Opening Remarks", Prof. Henry Wong's 60th Birthday Special Symposium, School of Chemical Biology and Biotechnology", Shenzhen, China, Nov. 21, 2010.
 29. C. Y. Ng, "The Role of Basic (Chemical) Research in Modern Society", Public Lecture, sponsored by Hong Kong Royal Society of Chemistry Lecture, the Chinese University of Hong Kong, Hong Kong, Dec. 2, 2010.
 30. C. Y. Ng, "Spectroscopy, Energetics, and Dynamics of Neutrals and Ions by High-Resolution VUV Photoionization and Photoelectron Methods", Pacific Chemistry Conference on "Frontiers in State-to-State Chemistry", Hawaii, Dec. 15-20-2010.
 31. C. Y. Ng, "Opening Remarks: International Workshop on Innovative Practices for Sciences and Nanotechnology Education", the Chinese University of Hong Kong, Hong Kong, Jan. 22, 2011.

32. C. Y. Ng, "Photoion-Photoelectron Studies by Vacuum Ultraviolet Lasers and Synchrotron Radiation", Chinese academy of Science, Shanghai, China, March 30, 2011.
33. C. Y. Ng, "Vacuum ultraviolet laser probes of chemical dynamics of aerospace relevance", AFOSR Contractor's Meeting, Pasadena, CA, May 15-17, 2011.
34. C. Y. Ng, "High resolution photoionization and photoelectron studies of radicals", Airlie Conference Center, DOE Contractor's Meeting, Warrenton, Virginia, May 31-June 3, 2011.
35. C. Y. Ng, "Spectroscopy of radicals and state-selected ion-molecule reaction dynamics by VUV laser photoion-photoelectron methods", XII National Chemical Dynamics Symposium Chengdu, Sichuan, China, June 10-13, 2011.
36. C. Y. Ng, "Spectroscopy and Dynamics of Ions and Neutrals by High-Resolution IR-VUV Two-Color Photoion-Photoelectron Methods", Department of Chemistry, National Tsing-Hua University, Taiwan, Nov. 9, 2011.
37. C. Y. Ng, "Benchmarking State-of-the-Art *Ab Initio* Thermochemical Predictions by High-Resolution Photoion-Photoelectron Measurements: From main group molecules to transition-metal compounds", Institute of Atomic and Molecular Sciences, Taipei, Taiwan, Nov. 10, 2011.
38. C. Y. Ng, "Absolute state-selected total cross sections for ion-molecule reactions of relevance to the ion chemistry of Titan: $N_2^+(X^2\Sigma_g^+; v^+ = 0-2, N^+=0-9) + CH_4$ (D_2 , H_2O , C_2H_2 , and C_2H_4)", "Titan Workshop", Miami Beach, March 11-14, 2012.
39. C. Y. Ng, "Benchmarking state-of-the-art *ab initio* thermochemical predictions by high-resolution photoion-photoelectron measurements from main group molecules to transition metal compounds", Conference on "Anharmonicity in medium-sized molecules and clusters", AMOC 2012, Paris-Est Marne-la-Vallée and Paris-Sud Universities, April 18-21, 2012.

B. Interactions

This project represents a collaborative project between our group at UC Davis and Dr. Y.-H. Chiu, Dr. Dale J. Levandier, James Dodd at the Hanscom Air Force Research laboratory. Dr. Albert Viggiano of the Hanscom Air Force Research Laboratory is also interested to collaborate with us to measure the vibrational energy distributions of product O_2^+ , NO^+ , and N_2^+ formed in the reactions of $O^+ + O_2$ (N_2), which are the most reactions occurring in planetary atmospheres.

C. Transitions

The thermochemical data obtained by our group based on VUV photoion and photoelectron measurements have been used by the "Active Thermochemical Table" project (project leader: Dr. Branko Ruscic) of the Argonne National Laboratory. We have recently extended these measurements to include transition metal species. Currently, the energetic predictions for transition metal-containing molecules are poor. Our measurements are expected to be valuable in guiding the further development of *ab initio* quantum calculation procedures.

X. New Discoveries:

None

XI. Honors/Awards:

Lifetime achievement honors

- 2009 Siu-Lien Wong Visiting Fellow, Chung Chi College, The Chinese University of Hong Kong
- 2005 Elected Fellow, American Association for Advancement of Science
- 2003 Distinguished Professor, UC Davis
- 1998 Alexander von Humboldt Senior Scientist Award
- 1997 Senior Fellow, Japanese Society for the Promotion of Science
- 1996 Distinguished Professor of Liberal Arts and Sciences, Iowa State University
- 1994 Iowa Regents Award for Faculty Excellence
- 1993 Elected Fellow, American Physical Society
- 1985 Honorary Professor of Chemistry, Zhengzhou University, China
- 1982 Camille and Henry Dreyfus Teacher-Scholar
- 1981 Alfred P. Sloan Foundation Fellow